User Interface Enhancements

In Creating and Modeling Experiments and Samples in the Refl1d Modeling Program

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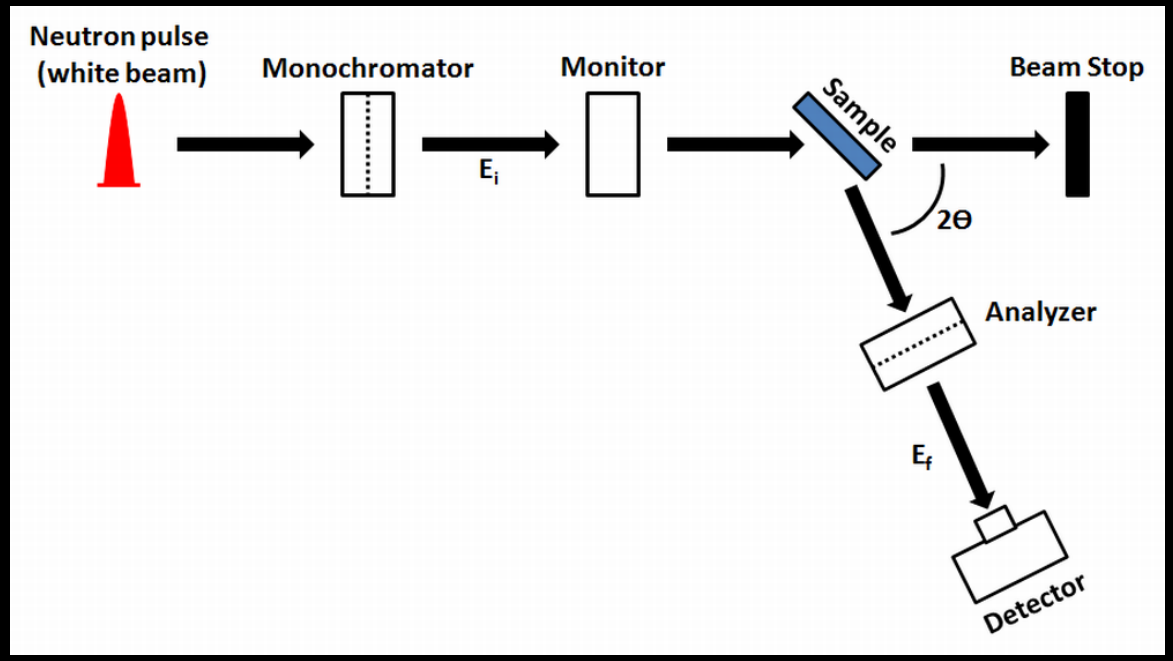
Motivation

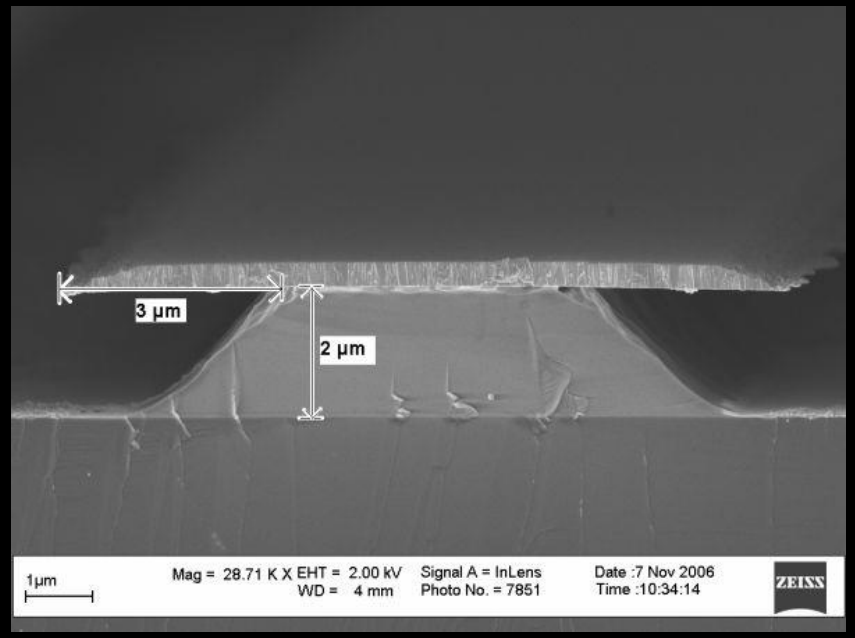
- We have a great program that is capable of doing a lot in the application of reflectometry, but accessing core features requires to much code fiddling.
- Minimize the time required to access core features of the program while also minimizing the user access and dependence on changing the code.

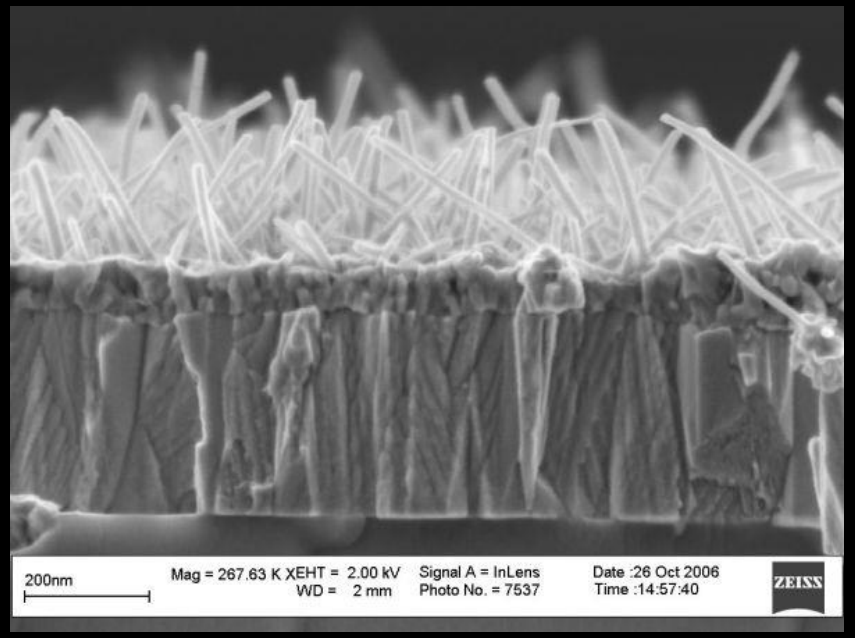
The Refl1d Program

- Observe the intensities of reflection as a function of the angle of incidence.
- “Fit” a model with data collected



Example: Tungsten Oxide

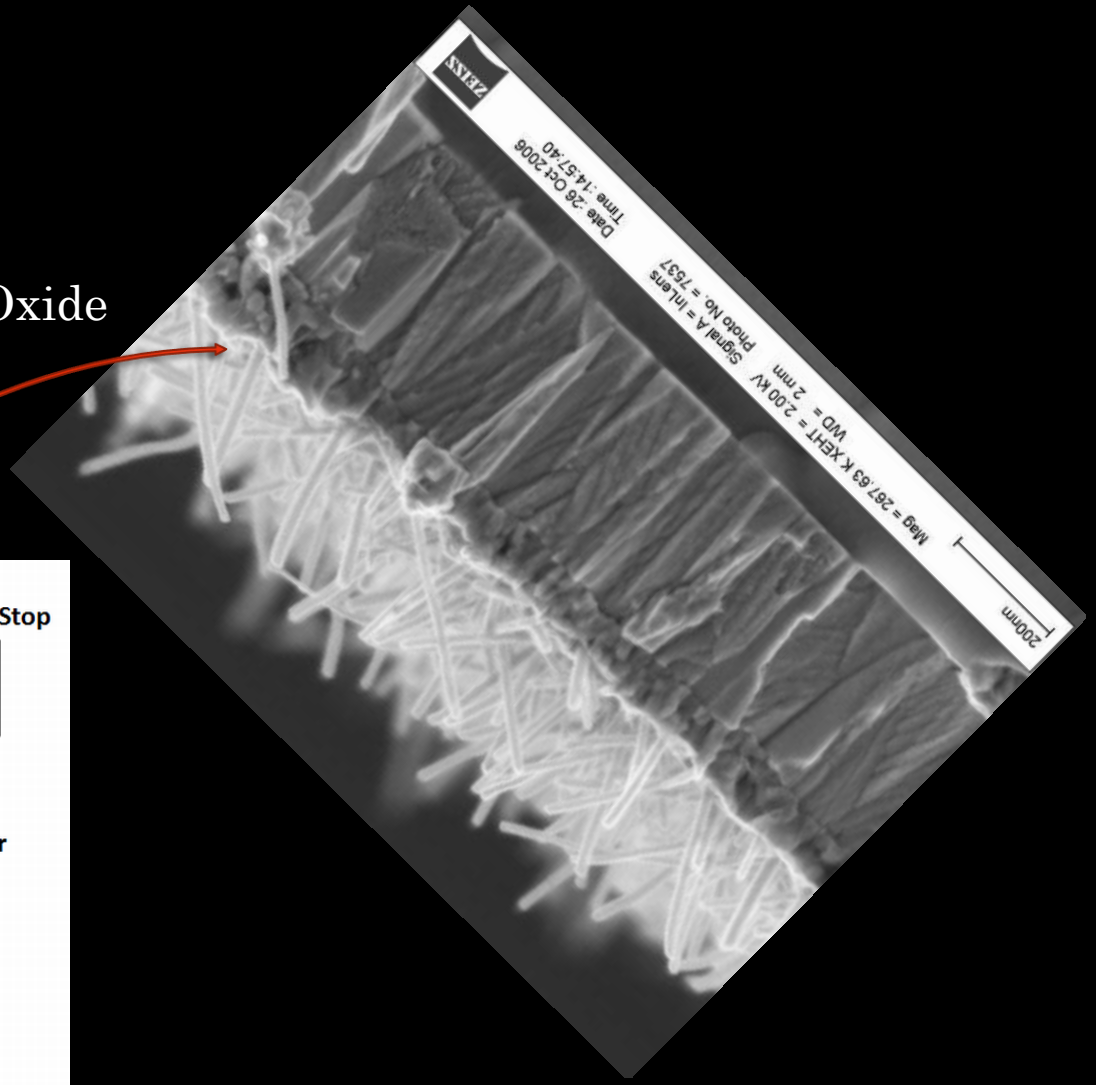


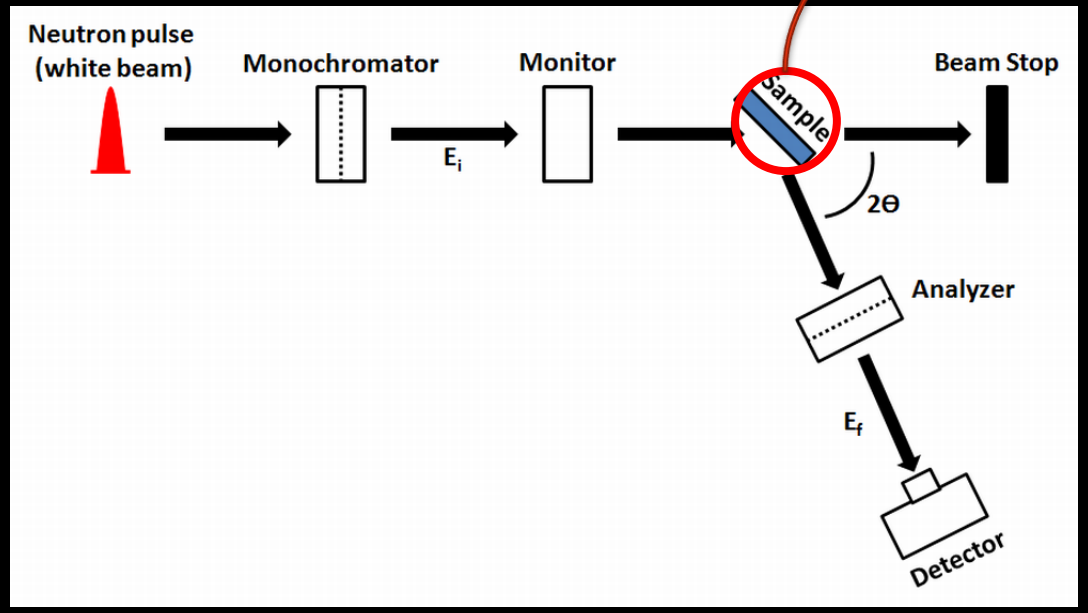


- Layer consists of a silicon substrate, with a free standing tungsten thin film and tungsten nano wires

Example

Tungsten Oxide





https://www.google.com/url?sa=i&rct=j&q=&esrc=s&source=images&cd=&cad=rja&uact=8&docid=-DLZH3SY8MikfM&tbnid=H4Fws81slLw34M:&ved=0CAUQjRw&url=http%3A%2F%2Fwww.intechopen.com%2Fbooks%2Fnanowires%2Fon-chip-tungsten-oxide-nanowires-based-electrodes-for-charge-injection&ei=YdHbU62yH9GUyASU4oCABw&bvm=bv.72197243,d.aWw&psig=AFQjCNFov6Y6x5YHsZ8YZtK3VkYut3EZ6A&ust=1407001300920466

What Refl1d needs

- The current way of editing layers requires the user to be familiar with the code.
  - Once the program has loaded and is running, there is no way to add, delete, or edit information about any of the layers in the stack.

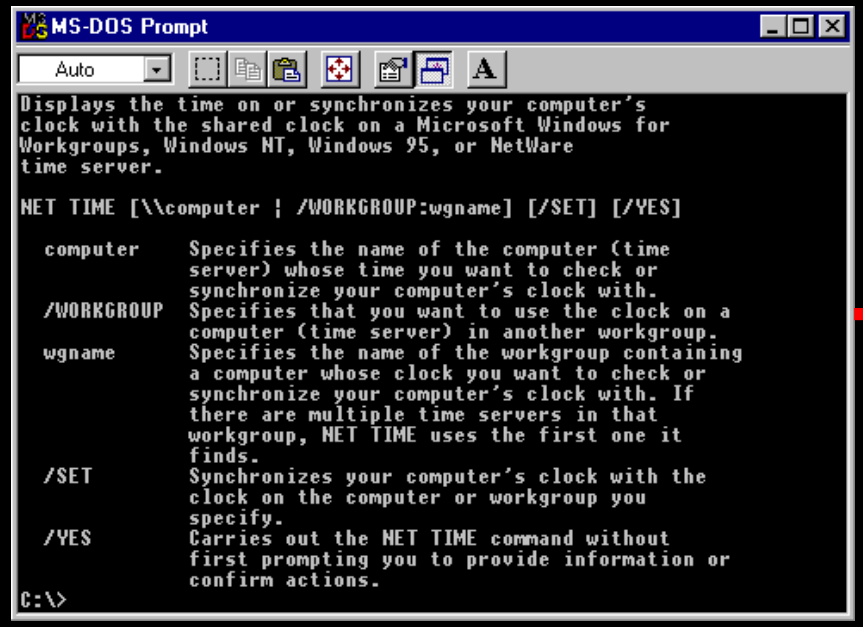
This made the current way of editing the layers in astack annoying

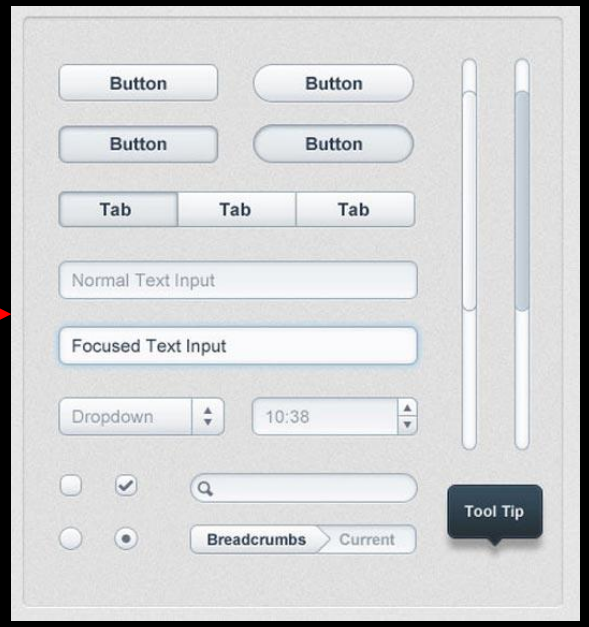
It is not friendly towards users and scientist who don't know how to program and just want to these sort of things to just "work"

Solution

Add a GUI (Graphical User Interface)

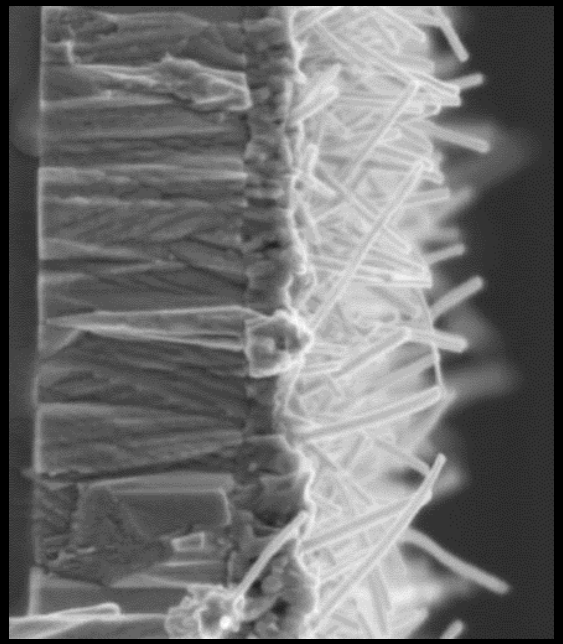
- We allow the users to do what they want by letting them right click in the program and work with the layers through a dialog.

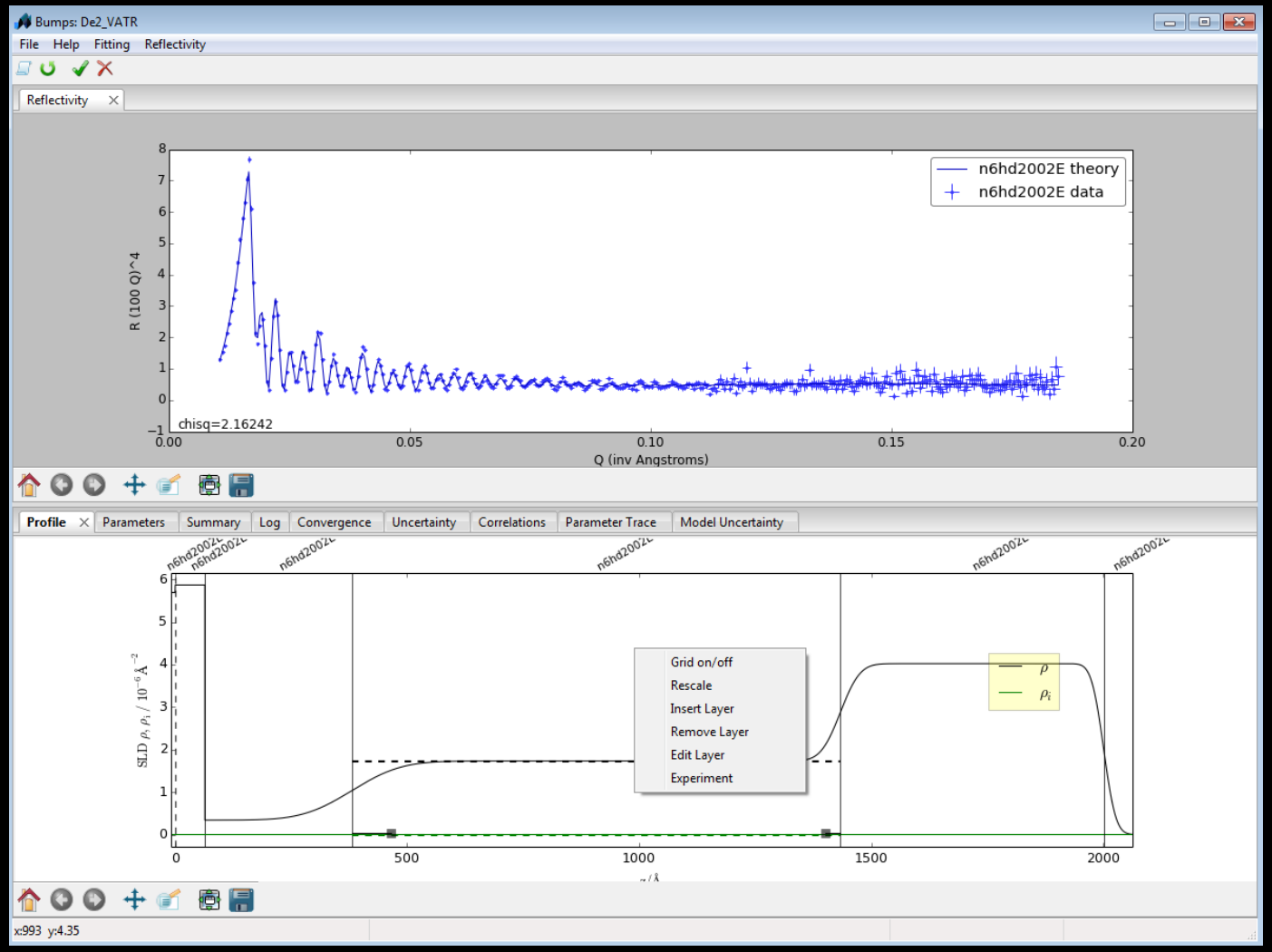




Invocating Pop Up Menu

- Invoke layer options by right clicking in the model view

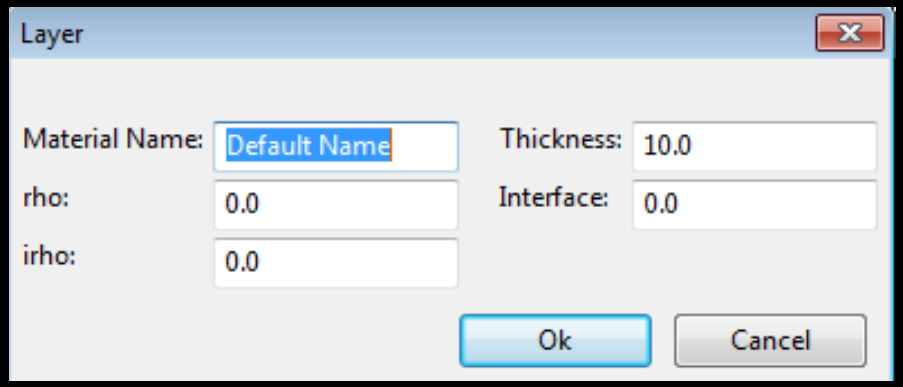


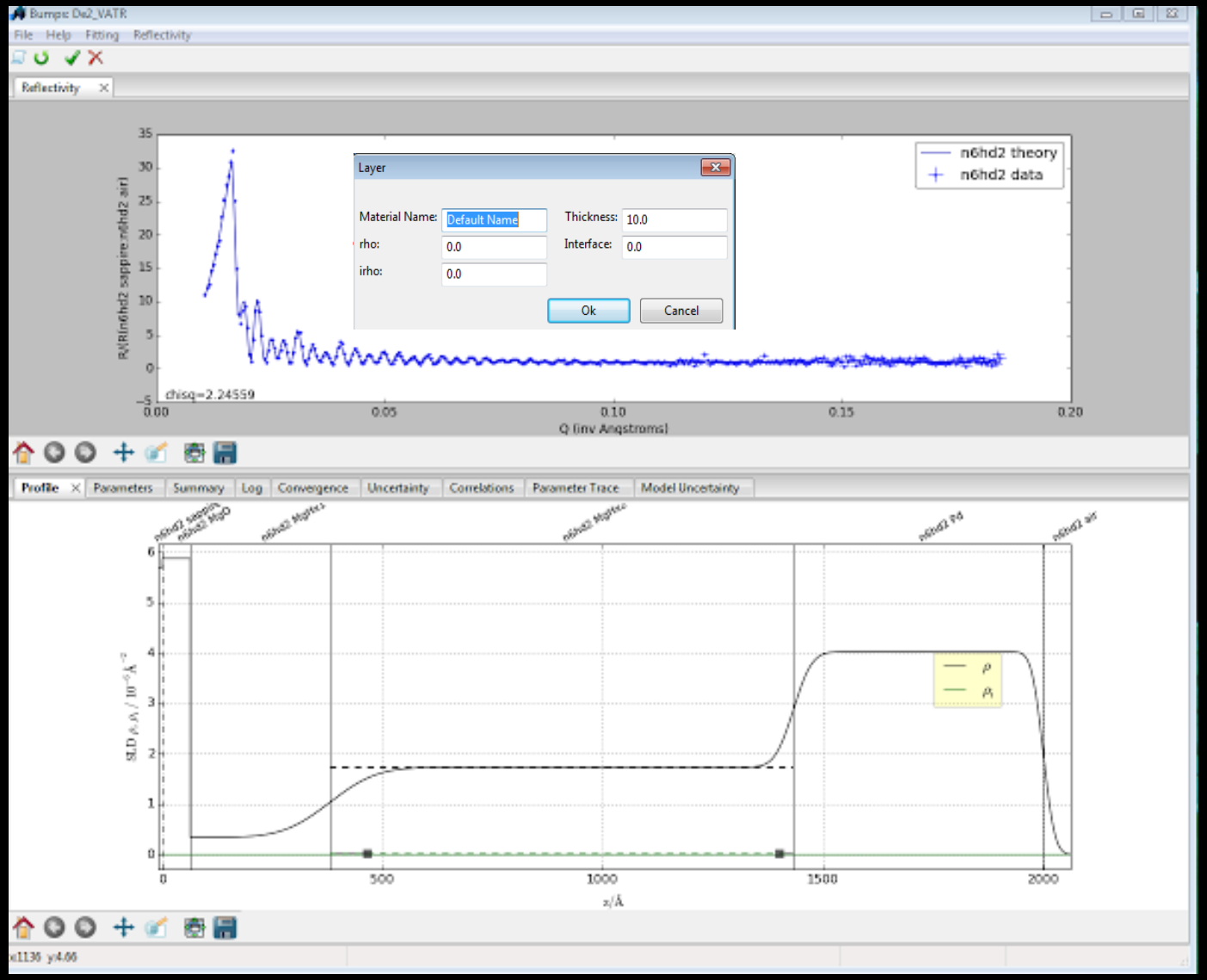


Inserting Layers

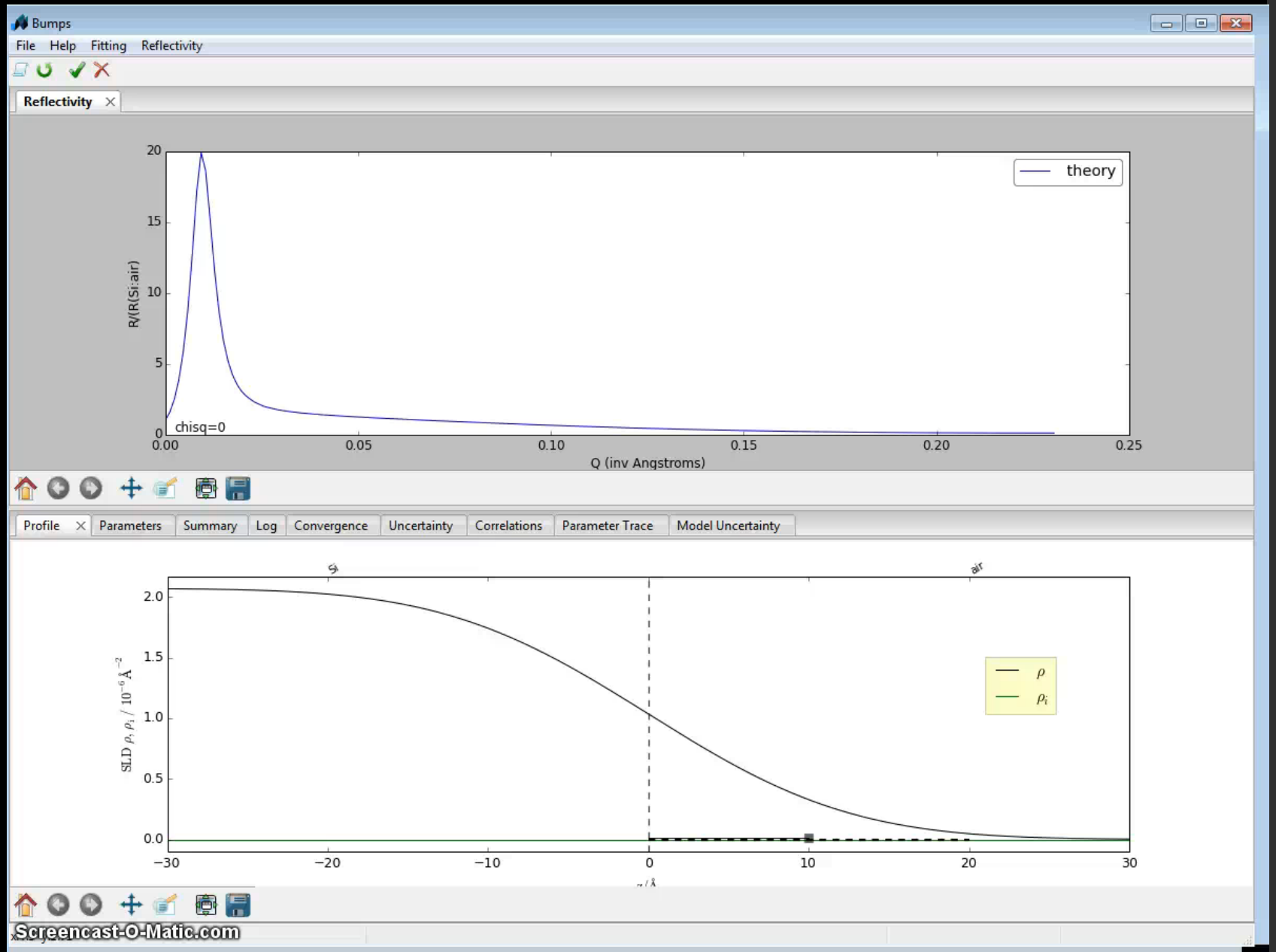
Available Parameters

- Material name
- Rho (scattering length density)
- iRho (imaginary SLD)
- Layer thickness
- Interface

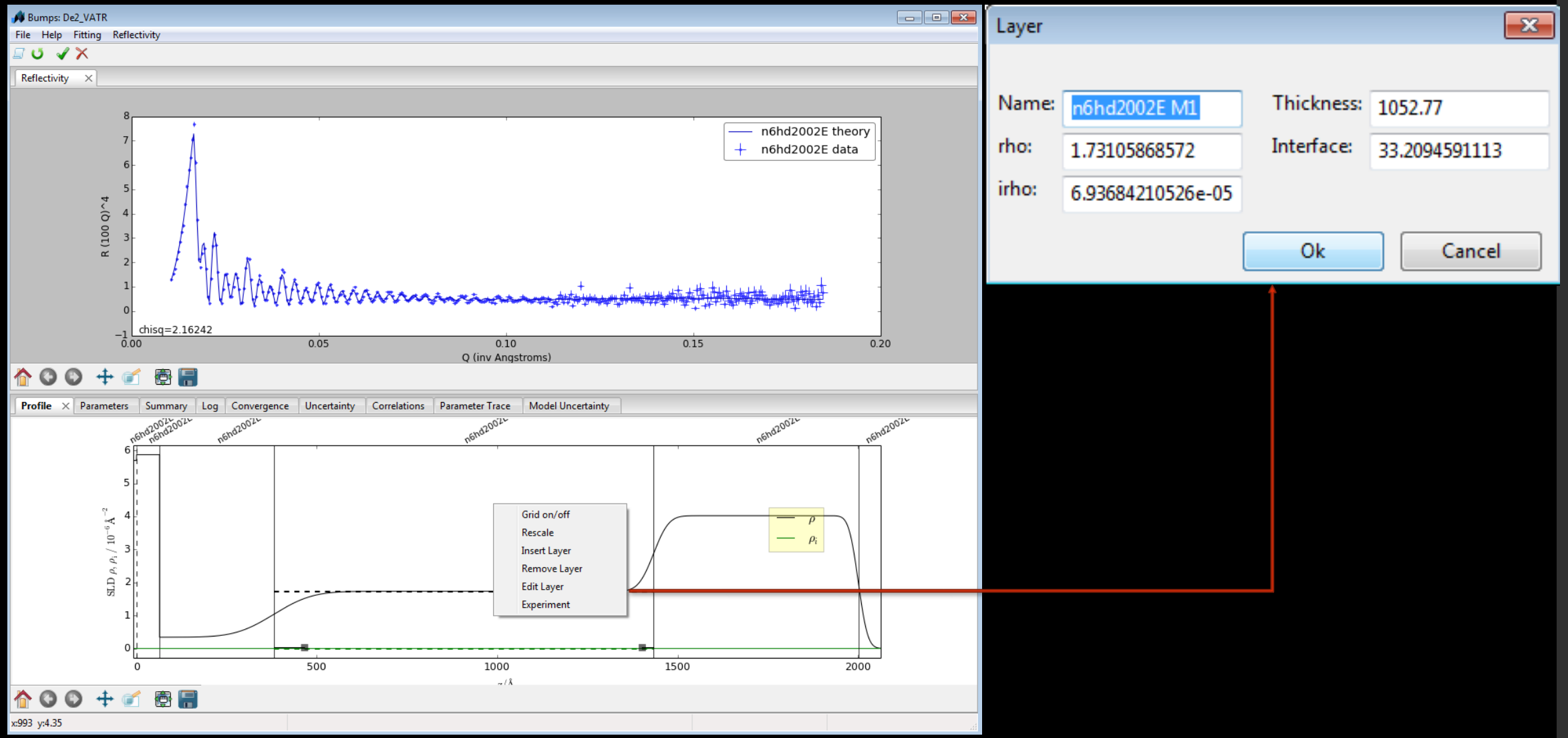




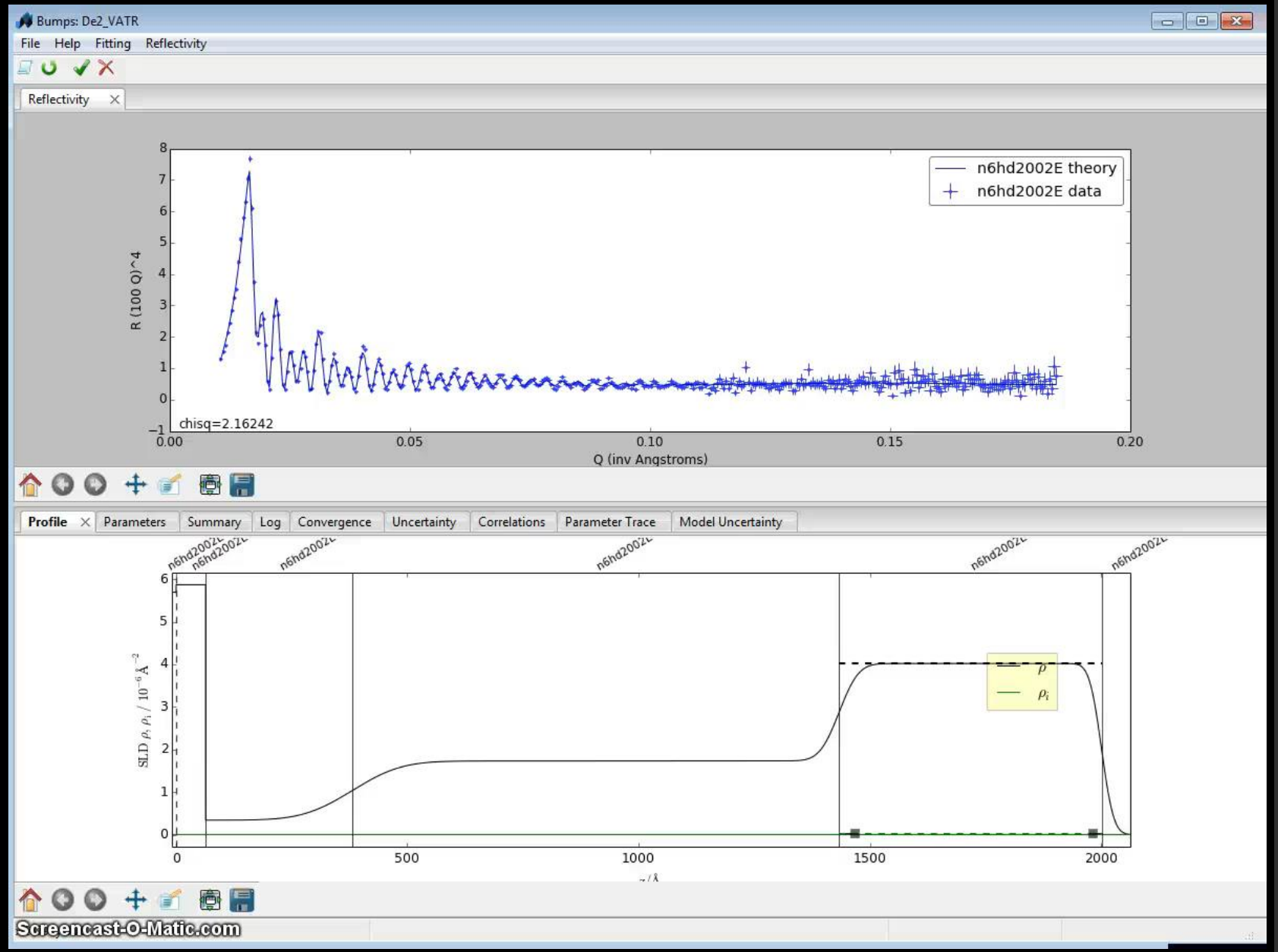
Demo


Bumps
File Help Fitting Reflectivity
Reflectivity
theory
chisq=0
R/(R(Si:air)
Q (inv Angstroms)
Profile Parameters Summary Log Convergence Uncertainty Correlations Parameter Trace Model Uncertainty
Si
air
SLD ρ, ρi / 10⁻⁶ Å⁻²
ρ
ρi
Screencast-O-Matic.com

Editing Layers



Demo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File Help Fitting Reflectivity
Reflectivity
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R (100 Q)^4
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Profile
Parameters
Summary
Log
Convergence
Uncertainty
Correlations
Parameter Trace
Model Uncertainty
SLD ρ_r / 10^{-6} Å^{-2}
ρ
ρ_i
Screencast-O-Matic.com

So Now What?

- Being able to create a model is good only if you can “model” it on an experiment (with actual data) and confirm that your model is accurate (via “fitting”)
- The current Refl1d does not allow the user to import an experiment in a fast and easy way in run time…

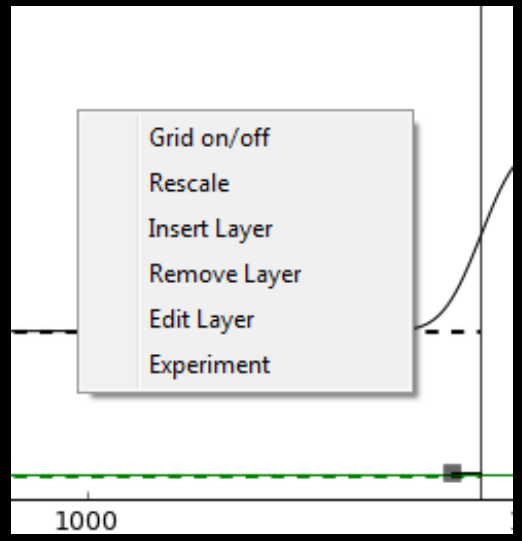
Solution

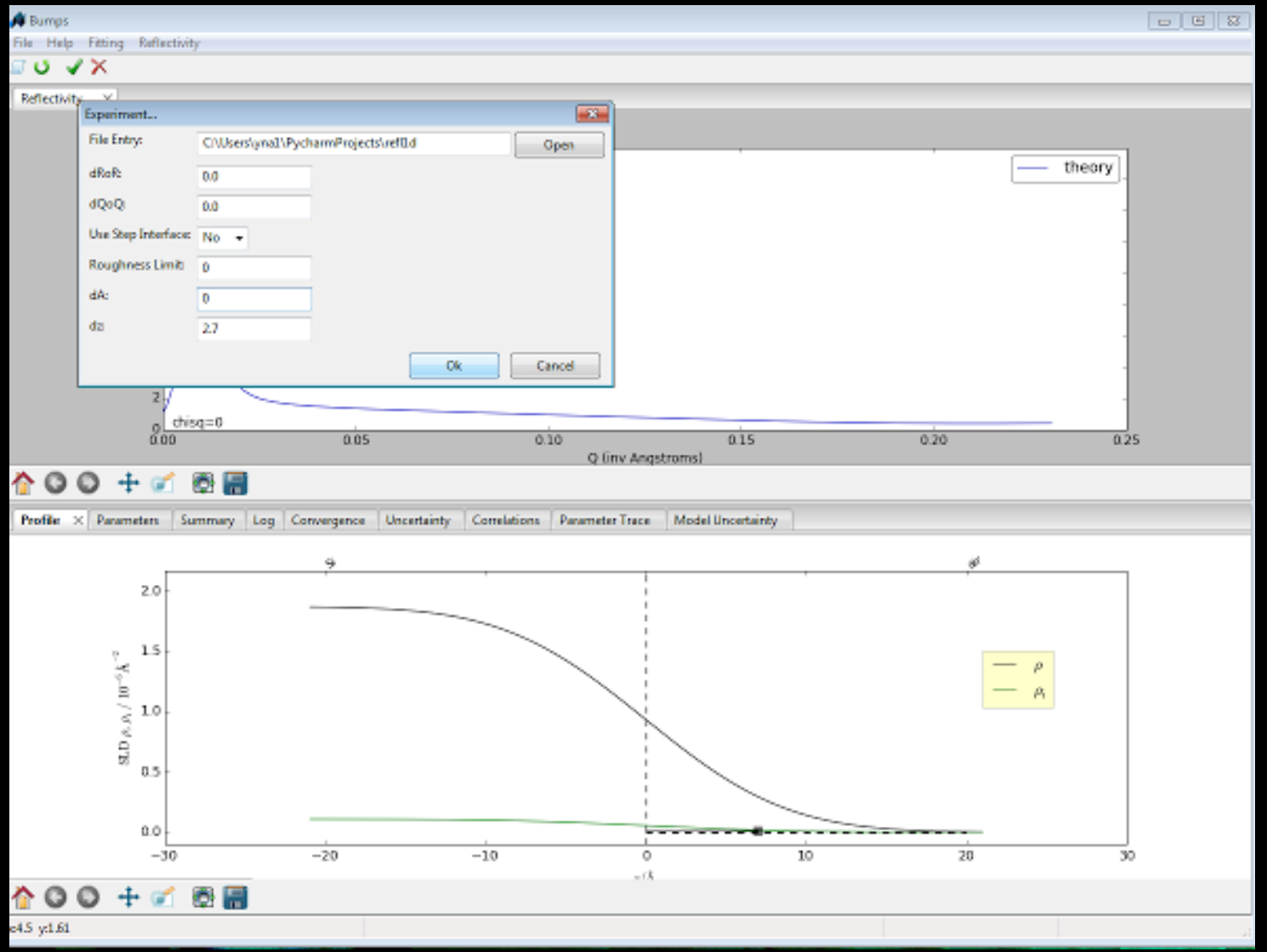
Enable the user to add data in runtime with through GUI (Graphical User Interface)

Experiment Dialog

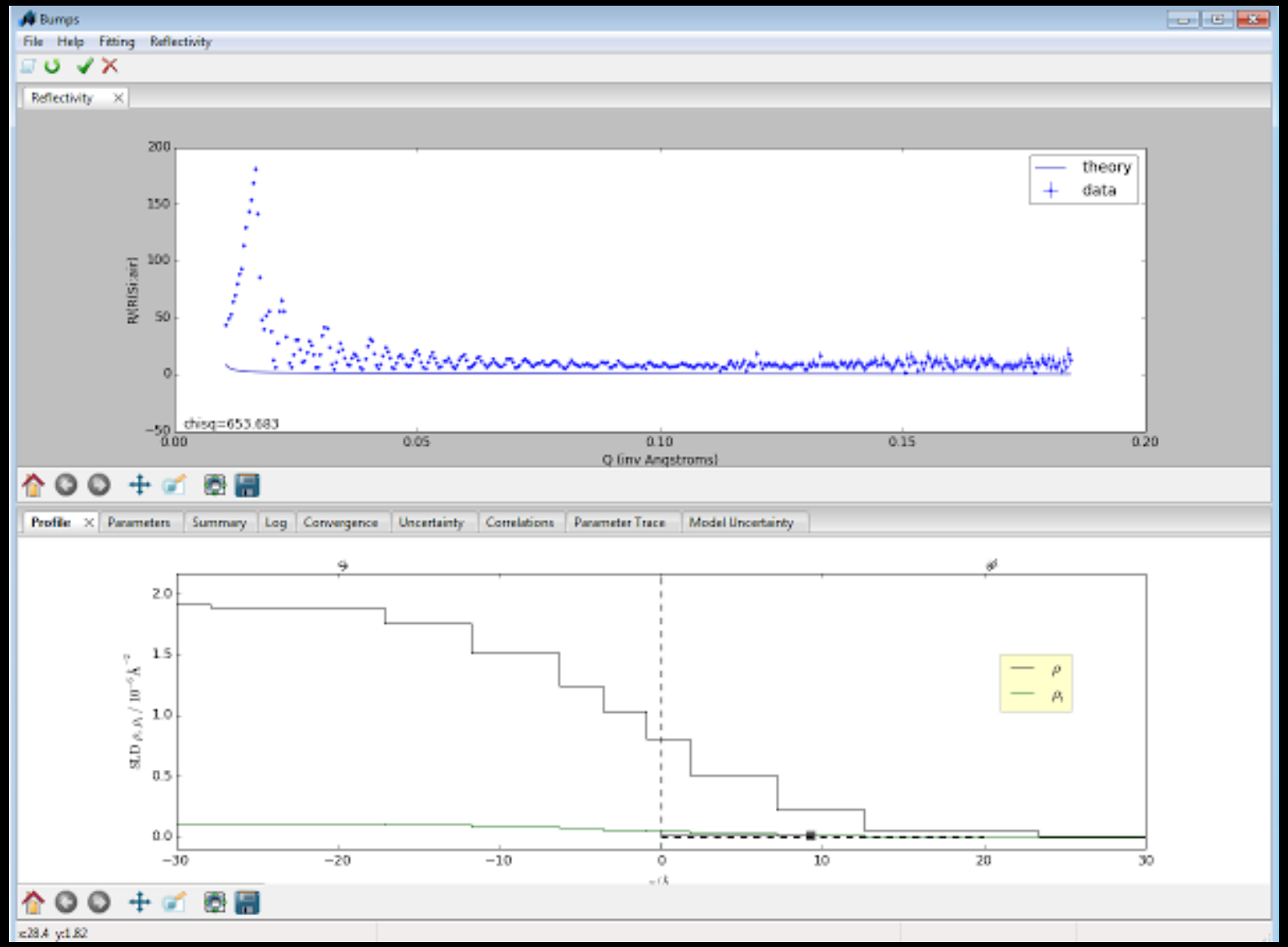
Available Parameters

- Data File
- dRoR (data uncertainty)
- dQoQ (data resolution)
- Step Interface
- Roughness Limit
- dA
- dz





Demo


Bumps
File Help Fitting Reflectivity
Reflectivity
theory
data
chisq=653.683
Q (inv Angstroms)
Profile
Parameters
Summary
Log
Convergence
Uncertainty
Correlations
Parameter Trace
Model Uncertainty

Conclusion

- We can now easily interact with the program in a much more user friendly way
- Scientist no longer need to edit the source code to access information about experiments and layers

Future Directions:

- More types of layers to edit
- Constraints between the layers

Acknowledgements

- Paul Kienzle
- Julie Borders
- Yamali Hernandez

Questions?